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NMR spectral and quantum-chemical structural study of phosphorinane derivatives

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Abstract

1. Nonempirical calculations were carried out for the first time for substituted phosphorinanes. The conformer with an axial methyl group at the phosphorus atom predominates in 5-methy--1,3,5-dioxaphosphorinanes as well as in the 5-oxa and 5-thio derivatives. The conformer with an equatorial methyl group at the phosphorus atoms and axial N-H bonds predominates in 5-thio-5-methyl-1,3,5-diazaphosphorinanes. 2. CNDO/2 and ab initio calculations for 5-methy--1,3,5-dioxaphosphorinanes and its 5-oxo derviatives show the same trend for change in the energies of the favored conformers. 3. The conformer with an axial phenyl group oriented approximately in the symmetry plane of the molecule predominates in 5-phenyl-1,3-5-dioxaphosphorinanes and their 5-oxo derivatives, while the conformer with an equatorial phenyl group oriented approximately in the molecular symmetry plane is favored in 1,3,5-triphenyl-1,3,5-diazaphosphorinane. © 1985 Plenum Publishing Corporation.

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